Elastic Moduli and Vibrational Modes in Jammed Sphere Packings

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Particles

Forces

Normal modes

Avalanches, plasticity, and nonlinear response in nonequilibrium solids

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Elastic response of amorphous solid

- Apply affine deformation on system
- In (one component) perfect crystal, particles follow the affine strain field
- In amorphous solid, force unbalance causes an additional relaxation

Affine deformation

Perfect lattice structure
⇒ Particles follow the affine strain field with no additional relaxation

Amorphous structure
⇒ Affine deformation causes force unbalance, driving an additional non-affine relaxation
Elastic response of amorphous solid

1. Deform the system affinely ⇒ rescale all coordinates $X \rightarrow X(1 + \gamma)$
2. **Force unbalances** are induced between particles
3. Undergo an additional non-affine relaxation $X(1 + \gamma) \rightarrow X'$

Elastic modulus = **Affine** + **Non-affine**

$$G = G_A - G_N$$

⇒ Non-affine relaxation decreases modulus (non-affine contribution)
Elastic response of amorphous solid

1. Deform the system affinely ⇒ rescale all coordinates $X \to X(1 + \gamma)$
2. **Force unbalances** are induced between particles
3. Undergo an additional **non-affine relaxation** $X(1 + \gamma) \to X'$

- **Forces** acting on particles induced by affine deformation
- **Particle displacements** driven by forces, during non-affine relaxation

During non-affine relaxation, **vibrational normal modes** are excited!
Vibrational normal modes – Density of states

- Harmonic potential
- Frictionless particles
- Crossover at $\omega^*$ from Debye-like regime to plateau regime
- On approach to jamming transition point $\varphi_c$, plateau regime extends towards zero frequency: $\omega^* \sim \Delta \varphi^{1/2} \to 0$

\[ \phi(r_{ij}) = \begin{cases} \frac{\varepsilon}{2} \left( 1 - \frac{r_{ij}}{\sigma} \right)^2 & (r_{ij} < \sigma) \\ 0 & (r_{ij} \geq \sigma) \end{cases} \]

Crossover frequency

\[ \Delta \varphi = \varphi - \varphi_c \]

L.E. Silbert et al., PRL (2005)
Vibrational normal modes – Polarization vector $e^k$

- **A, Debye-like regime**: Some plane-wave-like character
- **B, Plateau regime**: Filamentary nature of extended mode
- **C, High frequency regime**: Truely, highly localized mode

L.E. Silbert et al., PRE (2009)
A question in the present work

➢ Which vibrational normal modes play a role in energy relaxation process, during non-affine deformation?
Present particulate system

- 3 dimensional system
- Harmonic interaction
- Frictionless particles

\[ \phi(r_{ij}) = \begin{cases} \frac{\varepsilon}{2} \left(1 - \frac{r_{ij}}{\sigma}\right)^2 & (r_{ij} < \sigma) \\ 0 & (r_{ij} \geq \sigma) \end{cases} \]

- Close to jamming: Packing fraction \( \Delta \varphi = \varphi - \varphi_c = 10^{-1} \) to \( 10^{-6} \)

A, Debye-like regime:
\[ \omega < \omega^* \]

B, Plateau regime:
\[ \omega^* < \omega < \omega^h \]

C, High frequency regime:
\[ \omega > \omega^h \]

with characteristic frequencies
\[ \omega^* \sim \Delta \varphi^{1/2}, \quad \omega^h \sim 1 \]

L.E. Silbert et al., PRL(2005), PRE (2009)
Vibrational energy of normal mode

- Vibrational energy is separated into two components: (1) compressing/stretching energy and (2) sliding energy
- Sliding motion de-stabilizes the system: $-\delta E^k_\perp < 0$

$$\delta E^k = \frac{\omega^k}{2} = \delta E^k_\parallel - \delta E^k_\perp = \sum_{(i,j)} \left[ \frac{\phi''(r_{ij})}{2} e^k_{ij} \right]^2 + \frac{\phi'(r_{ij})}{2 r_{ij}} e^k_{ij} \bigg| e^k_{ij} \bigg|^2 \sim \Delta \varphi \times e^k_{ij} \bigg| e^k_{ij} \bigg|^2$$

(1) Compressing/Stretching

Compressing
$$e^k_\parallel \cdot n_{ij} < 0$$

Stretching
$$e^k_\parallel \cdot n_{ij} > 0$$

(2) Sliding

M. Wyart et al., PRE (2005)
Sliding motion and energy

- Sliding displacement and energy are independent of frequency

\[ e_{ij}^k \sim A^\perp \text{ (constant)} \]

\[ \delta E^k \sim \Delta \varphi e_{ij}^k \sim \Delta \varphi A^\perp \]

Graphs showing the behavior of \( e_{ij}^k \) and \( \delta E^k \) with respect to frequency. The graphs illustrate the independence of energy and displacement from frequency.
Compressing/stretching motions and energy

- At high frequencies, $\omega > \omega^*$
  \[ e^k_{ij} \sim \delta E^k_\parallel^{1/2} \sim \omega \]
  \[ \delta E^k_\parallel \sim \omega^2 / 2 \gg \delta E^k_\perp \]

- At low frequencies, $\omega < \omega^*$
  \[ e^k_{ij} \sim \Delta \varphi^{1/2} \omega^0 \]
  \[ \delta E^k_\parallel \sim \delta E^k_\perp \sim \Delta \varphi \omega^0 \]
Characterization of frequency $\omega^*$

At $\omega = \omega^*$, $\delta E^k \parallel \sim \frac{\omega^*}{2} \sim \delta E^k \perp \sim \Delta \phi$

$\omega^*$ is a point where the sliding energy starts to play a role!

$\delta E^k \parallel \approx \omega^2/2 \gg \delta E^k \perp \approx \omega^0$

$\sim \omega^{3/2}$
Normal-mode decomposition of non-affine modulus

Force field is induced by affine deformation

\[ \Sigma = \frac{\partial F}{\partial \gamma} \]

Non-affine displacements are driven by the force field

\[ \delta R_{na} = H^{-1} \cdot \Sigma \]

Energy relaxation (force times displacement) during the non-affine deformation

C.E. Maloney, PRL (2006)
Normal-mode decomposition of non-affine modulus

- Decompose non-affine modulus into each mode \( k \) contribution
- We can understand which modes play an important role in energy relaxation during non-affine deformation

**Force field** induced by affine deformation

\[
\Sigma = \sum_{k=1}^{3N-3} \Sigma^k e^k
\]

**Non-affine displacement** driven by force field

\[
\delta R_{na} = \sum_{k=1}^{3N-3} \delta R^k_{na} e^k = \sum_{k=1}^{3N-3} \frac{\sum^k}{\omega^k} e^k
\]

**Non-affine modulus**: Energy relaxation during non-affine deformation

\[
M_N = \frac{1}{V} \sum_{k=1}^{3N-3} M^k_N = \frac{1}{V} \sum_{k=1}^{3N-3} \Sigma^k \delta R^k_{na}
\]

Force field induced by affine deformation

Under (affine) shear deformation

- Force field is induced mainly along normal modes in the high frequency regime C: \( \omega > \omega^h \)
- Forces are related to compressing/stretching vibrational amplitude
- Crossover between A and B at \( \omega^* \) is caused by the sliding energy

\[ \sum_k \left( \approx \phi''(r_{ij}) e_{ij}^k \right) \]

\[ \sim \left\{ \begin{array}{ll}
\omega^0 & (\omega > \omega^h) \\
\omega & (\omega^* < \omega < \omega^h) \\
\omega^0 & (\omega < \omega^*)
\end{array} \right. \]
Non-affine displacement field (driven by force field) occurs mainly along normal modes in the Debye-like regime $A: \omega < \omega^*$

At $\omega < \omega^*$, the sliding energy drives the displacement field.

High frequency, energetic modes at $\omega > \omega^h$ are little excited.

\[
\delta R_{na}^k = \frac{\sum_k}{\omega^{k/2}}
\]

\[
\begin{cases} 
\omega^{-2} & (\omega > \omega^h) \\
\omega^{-1} & (\omega^* < \omega < \omega^h) \\
\omega^{-2} & (\omega < \omega^*) 
\end{cases}
\]
Force and displacement fields

**Force field:** Random distribution with short-range correlation

**Displacement field:** Vortex-like structure with long-range correlation

*Affine* vs *Non-affine* Stress-strain curve

**A** Plane-wave-like modes

**B** Filamentary extended modes

**C** Highly localized modes
Non-affine modulus – Energy relaxation

Non-affine modulus: Energy relaxation during non-affine deformation

\[ M_N^k = \sum_k \delta R_{\text{na}}^k \sim \begin{cases} 
\omega^{-2} & (\omega > \omega^h) \\
\omega^0 & (\omega^* < \omega < \omega^h) \\
\omega^{-2} & (\omega < \omega^*)
\end{cases} \]

A, Debye-like regime:
Energy relaxation is enhanced, due to the sliding motions

B, Plateau regime:
Mode contributions are independent of frequency

C, High frequency regime:
Few contributions
Our main conclusion

- Affine deformation induces the **force field** mainly along normal modes in the **high frequency regime C**.

- The force field drives the **non-affine displacement field** mainly along modes in the low frequency, **Debye-like regime A**.

- Energy relaxations (non-affine modulus) occur mainly in **Debye-like regime A and plateau regime B**, whereas those do not in regime C.

- In **Debye regime A**, the **sliding energy** destabilizes the system, inducing further energy relaxations.
Thank you for your attention

In collaboration with

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